**WISCONSIN**
UNIVERSITY OF WISCONSIN–MADISON

# CHEM 675 section 001 Syllabus
Introductory Quantum Chemistry

## COURSE INFORMATION

Introductory Quantum Chemistry
CHEM 675 001 ( 3 Credits )
2019-2020 Fall [1202]

### Description
Basic principles of quantum chemistry, exactly solvable problems, angular momentum, approximation methods, applications to electronic structure. Enroll Info: Chem 562 or consent of instructor

### Prerequisite(s)
CHEM 562 or graduate standing

### Instruction Mode
Classroom Instruction

### Section Level Com B
False

**Department:** CHEMISTRY
**College:** Letters and Science

## Canvas Course URL

https://canvas.wisc.edu/

⬛ **2019-2020 Fall [1202]**
**Term Start Date:** Wednesday, 4-Sep-2019  **Term End Date:** Friday, 10-Jan-2020

**Location and Schedule:** Chemistry Building 8335 MWF 9:55 AM-10:45 AM
**CRN:** 224002847

### How the Credit Hours are Met
This class meets for three 50-minute class periods each week over the semester and carries the expectation that students will work on course learning activities (reading, writing, problem sets, studying, etc) for about 2 hours out of classroom for every class period. The syllabus includes additional information about meeting times and expectations for student work.

## INSTRUCTORS AND TEACHING ASSISTANTS

### Instructor

⬛ EDWIN SIBERT
⬛ SIBERT@CHEM.WISC.EDU

## Instructor Availability

Room: 8305c
Time:  Mon. 1:30-2:30, Fri. 2:30-3:30

## GRADING AND COURSE MATERIALS

## Course Learning Outcomes (CLOs)

**1** Apply the laws of quantum mechanics to solve a range of problems of chemical interest
[S5977]

**2** Describe the energy levels of atomic systems using extensions of the quantum mechanical solutions to the hydrogen atom.
[S5978]

**3** Solve a variety of problems using the method of separation of variables especially the hydrogen atom.
[S5979]

**4** Justify the approximations that are made in order to obtain the quantum mechanical solutions for the electronic, vibrational, and rotational degrees of freedom of a diatomic molecule.
[S5980]

**5** Apply the concept of basis set expansions to solve for eigenvalues and eigenfunctions using basis sets.
[S5981]

**6** Apply perturbation theory appropriately to describe energy levels and wave functions of atomic and molecular systems.
[S5982]

**7** Predict the time evolution of observables, given solutions to the time independent Hamiltonian.
[S5983]

**8** Explain how one constructs both the time independent and time dependent Hamiltonian given the number of particles and the potential describing them.
[S5984]

**9** Explain with equations how and why transitions take place in atoms and molecules.
[S5985]

**10** Explain how normal modes are obtained and why they allow for a solutions of the molecular vibrations of polyatomic molecules.
[S5986]

**11** Understand angular momentum and the commutation properties of angular momentum operators.
[S5987]

## Grading

Your final course grade will be based on a 100 points scale. The total points are distributed as follows midterms (17 points each), problems sets (33 points), and final exam (33 points). If you receive 60 total points you will receive a B or better in this class. If obtain more than 75 total points you will receive an A. Your attendance in class is critical for sucess in this course, but is not part of you grade.

## Required Textbook, Software, & Other Course Materials

The textbook for this course is the fifth edition of `Quantum Chemistry' by Ira N. Levine. You can get used copies on Amazon at a reasonable price. You can probably find copies around the chemistry building if you are resourceful.

## EXAMS, QUIZZES, PAPERS & OTHER MAJOR GRADED WORK

### Exams, Quizzes, Papers & Other Major Graded Work

There are two in-class exams and a final. All exams are cumulative and are closed-book. The in-class exams are Wednesday on 10/16 and 11/13. The final exam is Dec 14 from 7:45AM - 9:45AM.

### Homework & Other Assignments

There will be 11 homework assignments. These assignment can be viewed by clicking on the "assignment" tab to the left. Homework is the most

important component of the class from a pedagogical point of view.  Assignments will be posted on Wednesdays and are due on the following Wednesday during class period.  You may discuss the homework with other students in the class, but you must turn in a single assignment for your group.    Problems sets are not accepted after class time on the day that they are due, so that I can discuss the solutions that day.    Some problems require the use of computer software.  You may use the software of your choice.  One of the choices is Excel.

## OTHER COURSE INFORMATION

Other Course Information

# Topics to be covered

1. Foundations of Quantum Mechanics and Particle in a Box (2 lectures) [Chapter 1-2]

2. Time Dependent Quantum Mechanics (1 lecture) [Chapter 2]

3. Piecewise Constant Potentials and Tunneling (2 lecture) [Chapter 2]

4. Operators, observables and a particle in a three-dimensional box (2 lectures) [Chapter 3]

5. The Harmonic Oscillator (3 lectures) [Chapter 4]

6. Central Force Problems and Angular Momentum (2 lectures) [Chapter 5]

7. Angular Momentum Operators (1 lecture) [Chapter 5]

8. Separation of Variables, center of mass variables, and the Hydrogen Atom (3 lectures) [Chapter 6]

9. More on the Foundations of Quantum Mechanics (2 lectures) [Chapter 7]

10. The Variational Principle (3 lectures) [Chapter 8]

11. He Atom and the Variational Principle  (1 lecture) [Chapter 9]

12. He Atom and Time Independent Perturbation Theory (2 lectures) [Chapter 9]

13. Spin, the Pauli Principle, and Hartree-Fock Theory (3 lectures) [Chapter 10-11]

14. Molecular Structure and the Born-Oppenheimer Approx. (4 lectures) [Chapter 13]

15. Molecular Rotations and Vibrations of Diatomic Molecules (3 lectures) [Chapter 13]

16. Molecular Rotations and Vibrations of Polyatomic Molecules (3 lectures)

17. Time Dependent Perturbation Theory (2 lectures) [Chapter 9]

18. Molecular Electronic Transitions (2 lectures)

## ACADEMIC POLICIES

### ACADEMIC INTEGRITY

By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison's community of scholars in which everyone's academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to https://conduct.students.wisc.edu/academic-integrity/

### ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES

**McBurney Disability Resource Center syllabus statement:** "The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA."
http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

### DIVERSITY & INCLUSION

**Institutional statement on diversity:** "Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals.

The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world." https://diversity.wisc.edu/